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Final Report LDRD 04-ERD-021

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FY06 LDRD Final Report

High strain-rate loading of nanocrystalline metals

LDRD project tracking code: 04-ERD-021

Eduardo Bringa, Principal Investigator

Abstract

In this project, we performed experiments and simulations to establish constitutive models for plastic behavior and to determine the deformation mechanism of nanocrystalline materials at different grain sizes (<100 nm) and high strain rates (>10^6/s). The experiments used both laser-induced shocks and isentropic compression to investigate, for the first time, the high-strain-rate deformation of nanocrystalline Ni. Samples were characterized using transmission electron microscopy, nanoindentation, profilometry, and x-ray diffraction before and after loading. We validated constitutive models using both atomistic molecular dynamics and continuum simulations performed at the boundary of their current computational possibilities to match experimental scales.

Introduction

Improved understanding of the deformation mechanisms of nanocrystalline metals could lead to the design of new materials with higher or lower resistance to plastic deformation. Nanocrystals are useful materials for laser targets and other applications due to their high hardness. Our simulations and experiments suggest a novel way to obtain even harder nanocrystals, both during and after shock loading. The results to date are unique because these strain rates had never before been attained in nanocrystals and because experiments and atomistic simulations cover the same length and time scales. Our use of local facilities (Janus laser, electron microscopy, characterization facilities, and massively parallel computers) increased in-house expertise.

Research Activities

We accomplished all planned milestones: a) loading, TEM and hardness measurements of about 20 samples; b) positron measurements of porosity; c) atomistic simulations of grain boundary sliding under pressure and of shocks in samples with grain sizes up to 50 nm; d) a new model of deformation was implemented into a continuum (micromechanics) code.

The results of the LDRD were reported in six high-profile publications, covering different aspects of our nanocrystal research.

The first publication of our LDRD [1] was an invited paper in a special issue on nanoscale materials in the *Journal of Metals*. We found scaling laws for the width of a shock wave propagating in a polycrystal. The irregularities in a shock front, that determine its width, can act as seeds for hydrodynamic instabilities and have to be avoided for a successful NIF capsule implosion.

Our highest impact paper [2], published in the journal *Science*, proposed a novel method to create ultra-hard nanocrystals, focusing on atomistic simulations results, and including preliminary experimental data to support this method. The details of the experiment for nanocrystalline Ni were later published in *Applied Physics Letters* [3]. We presented experimental results showing twinning in NiW nanocrystals in ref. [4].

In order to understand the detailed atomistic mechanism in this “ultra-hardening” of nanocrystals, we carried out controlled loading simulations that gave us a quantitative law to explain pressure-induced suppression of grain boundary sliding. This result was also published in *Applied Physics Letters* [5]. Such law was then applied inside a continuum-level code to calculate the mechanical behavior of nanocrystals under pressure [6]. This work, carried out in collaboration with a Los Alamos National Laboratory researcher, offers a pathway to build better constitutive models for polycrystals in general.

In addition to our publications, we had several conference presentations, including three at international conferences, as listed below [7-10].

Summary

During FY04-06 we obtained high-visibility publications (including one paper in Science, two in Applied Physics Letters, and one in Acta Materialia), a number of invited presentations, and press coverage of our results around the world. The deformation map that we obtained, together with our new continuum level model of grain boundary sliding fit to atomistic data, can be used to improve current continuum simulations and to plan future experiments involving polycrystals.

Our work (1) validated constitutive models (e.g., grain size and grain boundary corrections) important to the Stockpile Stewardship Program (SSP); (2) enhanced our understanding of nanocrystalline metals important to SSP; (3) mapped deformation processes at high strain rates; and (4) developed massively parallel simulation capabilities to study these processes. In addition, this project contributed to the Laboratory's mission in basic science.

References

LDRD publications

1. “Wave propagation in polycrystals”, E.M. Bringa, A. Caro, M. Victoria and N. Park, Journal of Metals **57**, 67-70 (2005). (UCRL-JRNL-213433)

2. “Ultra-hard nanocrystalline metals by shock loading”, E.M. Bringa *et al.*, Science, **309**, 1838 (2005). (UCRL-JRNL-213433)

3. “Deforming nanocrystalline nickel at ultrahigh strain rates”, Y.M. Wang, et al., Applied Physics Letters **88**, 061917 (2006). (UCRL-JRNL-213195)

4. “Deformation of nanocrystalline materials at ultrahigh strain rates-microstructure perspective in nanocrystalline nickel’, Y.M. Wang**,** E. Bringa, M. Victoria, A. Caro, J.M. McNaney, R. Smith, B.A. Remington, Journal De Physique IV **134**, 915-920 (2006). (UCRL-PROC-220628)

5. “Pressure effects on grain boundary plasticity in nanophase metals”, E.M. Bringa, E. Leveugle and A. Caro, Applied Physics Letters **89**, 023101 (2006). (UCRL-JRNL-330281)

6. “A viscoplastic micromechanical model for the yield strength of nanocrystalline materials”, R. Lebensohn, E.M. Bringa, and A. Caro, Acta Materialia **55**, 261 (2007). (UCRL-JRNL-219993).

Selected LDRD oral presentations:

7. “Shock-induced deformation mechanisms in nanocrystalline Ni”, Y.M. Wang et al., APS conference on Shock Compression of Condensed Matter, Baltimore, August 2005 (UCRL-PRES-214209).

8. “Deformation of nanocrystalline materials at ultrahigh strain rates”, Y.M. Wang et al., Dymat06, Dijon, France, April 2006 (UCRL-PRES-211450).

9. “Designing ultrahigh strength nanocrystals: making strong materials stronger”, E.M. Bringa *et al.*, Chemistry and Materials Sciences Directorate Review Committee, Livermore, May 2006 (UCRL-PRES-221467).

10. “Grain boundary sliding under pressure”, A. Caro et al., MRS meeting, December 2006 (UCRL-PRES-226328).